Time correlations and relaxation times for Hamiltonian systems

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Kubo's linear response theory

- Finite dimensional Hamiltonian system, endowed with the Gibbs measure (invariant)

$$H = H_0(x) \, , \quad \rho_0(x) = \frac{\exp(-\beta H_0(x))}{Z_0(\beta)} \, .$$

- A small perturbation $-hA(x)$ is introduced at time 0, $\rho(t,x) = \rho_0(x) + \Delta\rho(t,x)$.
- By Liouville's equation, with $B = \{A, H_0\}$,

$$\Delta\rho(t,x) = \beta h \int_0^t ds \, B(\Phi^s x) \, \rho_0(\Phi^s x)$$

- Expectation of the increment of a dynamical variable $C(x)$

$$\langle \Delta C \rangle(t) = \beta h \int_0^t ds \int_{\mathcal{M}} dx \, C(\Phi^{-s} x) B(x) \, \rho_0(x)$$

Time correlations: definitions and power series of time

Consider a Hamiltonian system on the phase space $\mathcal{M}$, with an invariant probability measure μ, and a function $f \in L^2(\mu, \mathcal{M})$.

$$\mathbf{C}_f(t) \stackrel{\text{def}}{=} \int_{\mathcal{M}} d\mu(x)\, f(x) f(\Phi^{-t}x) - \left(\int_{\mathcal{M}} d\mu(x)\, f(x) \right)^2 \; .$$

One has $|\mathbf{C}_f(t)| \le \mathbf{C}_f(0) = \sigma_f^2$.

There exists a series expansion in powers of t, as a function of the successive derivatives of f with respect to the flow, $f^{(k)} \stackrel{\text{def}}{=} \{f^{(k-1)}, H\}$, $f^{(0)} \stackrel{\text{def}}{=} f$. If $f^{(k)} \in L^2(\mu, \mathcal{M})$ for $k \le n$,

$$\mathbf{C}_f(t) = \sigma_f^2 + \sum_{k=1}^{n} (-1)^k \|f^{(k)}\|_{L^2}^2 \frac{t^{2k}}{(2k)!} + \\ (-1)^{n+1} \int_0^t dt_1 \cdots \int_0^{t_{2n-1}} dt_{2n} \, \|f^{(n)}(\Phi^{-t_{2n}}x) - f^{(n)}(x)\|_{L^2}^2$$

Finite time behaviour and relaxation times

The definite sign of the remainder enables us to define a sensible lower bound for the relaxation times of the considered system (in response to a given perturbation).
In particular, as for $n = 1$,

$$\mathbf{C}_f(t) \geq \sigma_f^2 - \|\{f, H\}\|_{L^2}^2 \frac{t^2}{2} \ ,$$

up to times of order $\sigma_f / \|\{f, H\}\|_{L^2}$ the system is far from having relaxed.

Analogue of the stability times of perturbation theory, but we need only probabilistic estimates: it is possible to attain the thermodynamic limit.

Asymptotic behaviour: connection with Stieltjes moment problem

Consider the Laplace transform $F(s)$ of $\mathbf{C}_f(t)$. Formally,

$$F(s) = \int_0^\infty dt \left(\sum_{n=0}^{\infty} (-)^n \frac{c_n}{(2n)!} t^{2n} \right) e^{-st} = \sum_{n=0}^{\infty} (-)^n \frac{c_n}{s^{2n+1}} \ , \qquad (1)$$

where $c_n = \|f^{(n)}\|^2_{L^2}$.

The r.h.s. is an asymptotic expansion of $F(s)$, but Stieltjes, in a beautiful work, studied convergent continued fraction expansions for series of this kind, and discovered the connection with the moment problem which now bears his name.

We formulate the result as a function of the spectral measure $\alpha(\omega)$ for the correlations:

$$\mathbf{C}_f(t) = \frac{1}{2} \int_{-\infty}^{+\infty} e^{i\omega t} d\alpha(\omega) \ .$$

Proposition (Stieltjes)

Let $\mathbf{C}_f(t)$ be analytic in t about the origin and continuous for any $t \in \mathbb{R}$.

- *$F(s)$ is analytic in the half plane Re $s > 0$ and*

$$F(s) = s \int_0^{+\infty} \frac{d\alpha(\omega)}{s^2 + \omega^2} ,$$

- *The continued fraction which approximates the r.h.s. of (1) converges to $F(s)$ for Re $s > 0$ and the Borel positive measure $\gamma(u) = \alpha(\sqrt{u})$ solves the Stieltjes moment problem for the coefficients c_n.*

Exponential decay of correlations and poles

Corollary

$\mathbf{C}_f(t)$ *decays exponentially fast if and only if the* c_n *are such that the distribution function* $\alpha'(\omega)$ *exists and* $\alpha'(\omega) = 2\sqrt{u}\,\gamma'(u)$ *is analytic.*

Extremely complicated to get this information: there are works by Akhiezer and Krein on the existence of the distribution function for the Hamburger moment problem, work by Hausdorff for “his” moment problem. Sharp control on c_n is needed.

It is easier to get some indications on the presence of poles of $F(s)$ (finite jumps for α) $\longrightarrow$ sufficient condition for a sub-exponential decay.

Numerical investigations

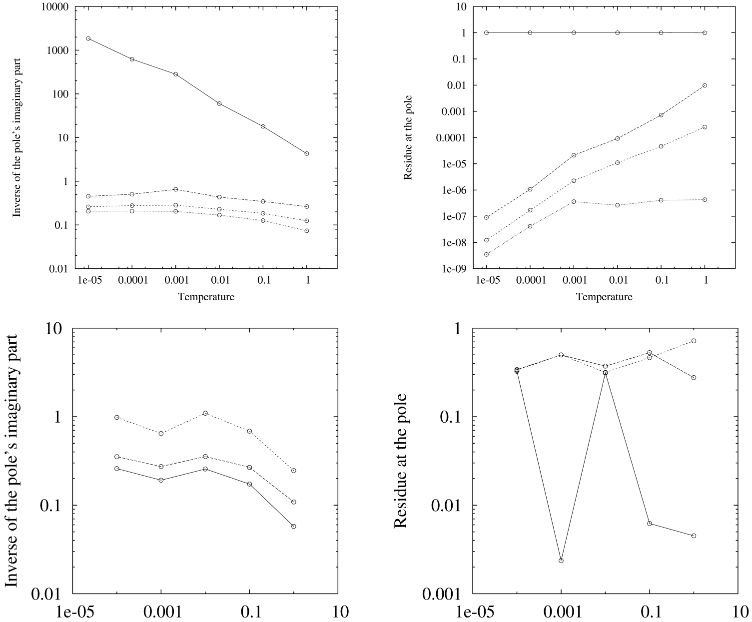
Rational approximation for the series (1), as

$$F_{2n}(s) = s\frac{P_{2n}(s)}{Q_{2n}(s)} = s\sum_{k=0}^{n}\frac{\rho_k}{s^2+\omega_k^2} \ ,$$

where the ω_k and ρ_k at order $2n$ depend only on the coefficients c_k, for $k \le 2n$.

Numerical test on the celebrated FPU-model. Two quantities of interest, energy of the low frequency normal modes $\mathcal{E}$ and kinetic energy of half of the chain $\mathcal{K}$.

Study for different values of the temperature T, entering the Gibbs measure.



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